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A conservative quaternion-based time integration algorithm for rigid body rotations with implicit constraints

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Summary. A conservative time integration algorithm for rigid body rotations is presented in a purely algebraic form in terms of the four quaternions components and the four conjugate momentum variables via Hamilton's equations. The introduction of an extended mass matrix leads to a symmetric set of eight state-space equations where constraints are embedded without explicit use of Lagrange multipliers. The algorithm is developed by forming a finite increment of the Hamiltonian, which defines the proper selection of increments and mean values that leads to conservation of energy and momentum. The accuracy and conservation properties are illustrated by examples.

Key words: finite rotations, quaternion parameters, conservative integration

Introduction

Time-integration of rigid body motion is of interest in numerous applications in engineering. Conservative integration procedures derived from an integrated form of the equations of motion are particularly attractive since they can be designed to provide energy and momentum conserving schemes, see e.g. [1] or [2]. However, the integration of finite rotations is complicated by the fact that they do not obey simple vector addition rules.

In this paper, a conservative time-integration algorithm for rigid body rotations is presented in terms of the four-component unit quaternions as this allows for a purely algebraic format without singularities. The governing equations are derived from the finite increment of the Hamiltonian in terms of the quaternion parameters and their four-component conjugate momentum vector yielding a symmetric set of eight state-space equations similar to [3]. However, the present formulation illustrates that the Lagrange multiplier - initially introduced in connection with the quaternion normalization constraint - can be eliminated by introduction of a projection operator in front of the load potential gradient. Furthermore, the formulation makes use of an extended mass matrix and role of the auxiliary inertia parameter is identified as an enforcing multiplier on the normalization constraint.

Equations of rigid body motion

Unit quaternions or Euler parameters are characterized as a four component quantity composed by a scalar part q_0 and a vector part $\boldsymbol{q}$ in the form

$$\mathbf{q}^T = [q_0, \boldsymbol{q}^T]. \tag{1}$$

Only three independent parameters are required for describing three-dimensional rotations, and thus the four quaternion parameters are redundant and satisfy the normalization constraint

$$\mathbf{q}^T\mathbf{q} - 1 = 0. \tag{2}$$

A particularly attractive feature of the quaternion representation of rotations is that the angular velocity is a bi-linear form in terms of the quaternion $\mathbf{q}$ and its time-derivative $\dot{\mathbf{q}}$, hence the kinetic energy can be expressed in the bi-quadratic format

$$\mathcal{T} = \tfrac{1}{2}\boldsymbol{\Omega}^T\mathbf{J}\,\boldsymbol{\Omega} = \tfrac{1}{2}\,\dot{\mathbf{q}}^T\,\mathbf{M}(\mathbf{q},\mathbf{q})\dot{\mathbf{q}}, \tag{3}$$

Here, an augmented inertia matrix $\mathbf{J} = \mathrm{diag}[J_0, \boldsymbol{J}]$ is introduced with the auxiliary parameter $J_0 > 0$. This leads to a non-singular 4×4 mass matrix $\mathbf{M}(\mathbf{q},\mathbf{q}) = 4\,\mathbf{Q}(\mathbf{q})\,\mathbf{J}\,\mathbf{Q}(\mathbf{q})^T$ where $\mathbf{Q}(\mathbf{q})$ denotes the orthogonal 4×4 matrix associated with quaternion pre-multiplication with $\mathbf{q}$. Several proposals for a specific value of J_0 based on physical reasoning have been given in the literature, e.g. [3]. However, the following examples demonstrate its role as a multiplier on the normalization constraint (2) rather than a physical parameter.

The conjugate four-component momentum vector follows as the partial derivative of the kinetic energy $\mathcal{T}$ with respect to $\dot{\mathbf{q}}$ as

$$\mathbf{p} = \frac{\partial\mathcal{T}}{\partial\dot{\mathbf{q}}^T} = \mathbf{M}(\mathbf{q},\mathbf{q})\,\dot{\mathbf{q}}, \tag{4}$$

and is easily shown to satisfy the following orthogonality constraint

$$\mathbf{q}^T\mathbf{p} = 0. \tag{5}$$

This can be used to prove the alternative representations of the kinetic energy

$$\mathcal{T} = \tfrac{1}{2}\,\mathbf{p}^T\,\mathbf{M}^{-1}(\mathbf{q},\mathbf{q})\,\mathbf{p} = \tfrac{1}{2}\,\mathbf{q}^T\,\mathbf{M}^{-1}(\mathbf{p},\mathbf{p})\,\mathbf{q}, \tag{6}$$

where the roles of $\mathbf{q}$ and $\mathbf{p}$ can be interchanged without changing the value of the total product.

Hamilton's equations is a convenient starting point for deriving the equations of motion for rigid body rotations and can be expressed as the two first-order differential equations

$$\dot{\mathbf{q}} = \frac{\partial\mathcal{H}}{\partial\mathbf{p}^T}, \qquad \dot{\mathbf{p}} = -\frac{\partial\mathcal{H}}{\partial\mathbf{q}^T}. \tag{7}$$

In the present formulation it is advantageous to use an augmented form of the Hamiltonian, where the normalization constraint (2) initially is included via a Lagrange multiplier λ

$$\mathcal{H} = \mathcal{T}(\mathbf{q},\mathbf{p}) + \mathcal{V}(\mathbf{q}) + \lambda(\mathbf{q}^T\mathbf{q} - 1), \tag{8}$$

and where it is assumed that the external forces can be derived from a potential $\mathcal{V}(\mathbf{q})$.

The equations of motion then follow by differentiation of (8) using either of the bi-quadratic expressions for the kinetic energy (6). Hereby the kinematic and dynamic equations of motion are obtained as

$$\dot{\mathbf{q}} = \quad \mathbf{M}^{-1}(\mathbf{q},\mathbf{q})\,\mathbf{p} \tag{9a}$$

$$\dot{\mathbf{p}} = -\mathbf{M}^{-1}(\mathbf{p},\mathbf{p})\,\mathbf{q} \;-\; \partial\mathcal{V}/\partial\mathbf{q}^T \;-\; 2\lambda\mathbf{q}. \tag{9b}$$

In addition, differentiation with respect to the Lagrange multiplier gives the normalization constraint (2).

A crucial step in the present formulation is that the Lagrange multiplier can be eliminated by using the time-derivative of the orthogonality condition (5) given by

$$\mathbf{q}^T\dot{\mathbf{p}} + \mathbf{p}^T\dot{\mathbf{q}} = \; -\mathbf{q}^T\big(\partial\mathcal{V}/\partial\mathbf{q}^T + 2\lambda\mathbf{q}\big) = 0. \tag{10}$$

This determines the Lagrange multiplier and substitution into the dynamic equation (9b) yields

$$\dot{\mathbf{p}} = -\mathbf{M}^{-1}(\mathbf{p},\mathbf{p})\,\mathbf{q} \;-\; \Big(\mathbf{I} \;-\; \frac{\mathbf{q}\,\mathbf{q}^T}{\mathbf{q}^T\mathbf{q}}\Big)\frac{\partial\mathcal{V}}{\partial\mathbf{q}^T}. \tag{11}$$

It is seen that the effect of eliminating the Lagrange multiplier essentially corresponds to introducing a projection operator in front of the external potential gradient that eliminates any component proportional to $\mathbf{q}$. Hereby the time-derivative of the orthogonality constraint (5) is satisfied for any external potential $\mathcal{V}$. In addition, it is easily verified that the time-derivative of the normalization constraint (2) is contained in the kinematic equation (9a) by pre-multiplication with $\mathbf{q}^T$ and utilization of the orthogonality condition (5).

An energy and momentum conserving time-integration algorithm can be obtained by deriving the discretized form of the equations of motion via the finite increment of the augmented Hamiltonian over the time interval Δt. The kinetic energy (6) is a symmetric quadratic form, and thus the increment can be expressed as twice the product of the increment of the first factor and the mean value of the other factor. The potential gradient is introduced via its finite derivative $\partial\mathcal{V}^*/\partial\mathbf{q}$, and the Lagrange multiplier is eliminated by using the incremental form of (5) analogous to the equivalent continuous system. This ensures, that the two original time-dependent constraint conditions are contained in the discrete equations of motion via their increments, and thus, if the constraints are satisfied initially, they will also be satisfied at any later time step without recourse to Lagrange multipliers.

Examples

The accuracy and conservation properties are illustrated by considering two examples: First a freely rotating box is considered. The geometry and parameters are given in [2], and the motion is initiated as unstable rotation around its intermediate axis of inertia with a small perturbation.

The local components of the angular velocity are illustrated in Fig. 2. Initially the box rotates around the global x_3-axis. At time $t = t_1$ the box tips over approaching a preliminary state with rotation about the initial rotation axis turned upside down, and at time t_3 the box returns to its initial configuration. This behavior is repeated in a periodic manner. While the kinetic energy, the global components of the angular momentum and the magnitude of the local angular momentum are conserved within a relative error of 10^{-12}, the algorithm exhibits a second-order period error. This can be evaluated as the difference between two turning points in

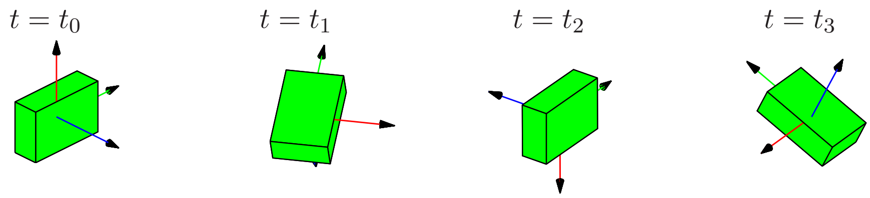

Figure 1. Motion of box at selected time steps, $\Delta t = 0.01$.

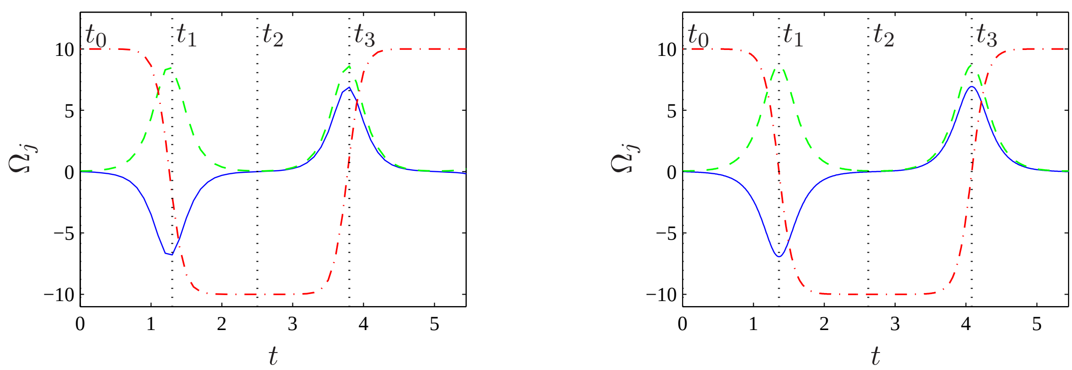

Figure 2. Local angular velocity components Ω_1 (—), Ω_2 (- -), Ω_3 (-·-). (a) $\Delta t = 0.1$, (b) $\Delta t = 0.01$.

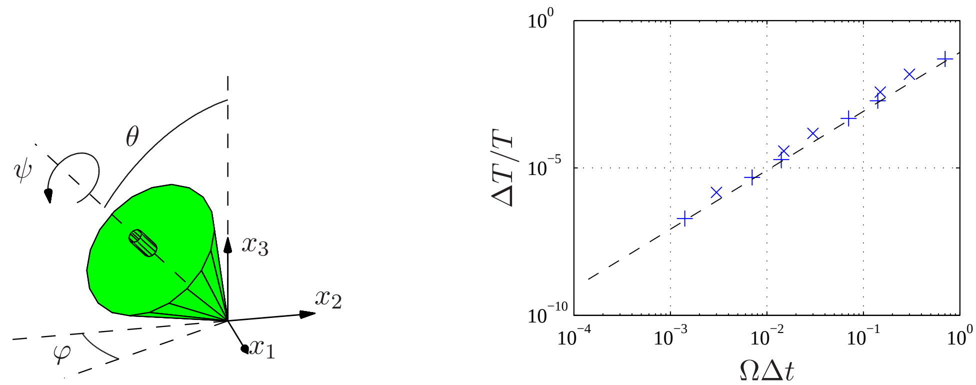

Figure 3. (a) Configuration of rotating top. (b) Relative period error. Precessing top (+), Fast top (×), $(\Omega\Delta t)^2/12$ (− −).

Fig. 2(a) and 2(b) corresponding to a shortening in time scale of approximately 8% when using $\Delta t = 0.1$. Furthermore, simulations illustrate that the error on the normalization constraint (2) decreases roughly in proportion to the increase in J_0, while the orthogonality constraint (5) is satisfied within the numerical accuracy irrespective of value of J_0.

The second example considers the motion of a top in a gravitational field with one point fixed. The motion is characterized in terms of the nutation angle θ, the precession angle φ and the spin angle ψ as illustrated in Fig. 3(a). The dimensions correspond to the ones used in [3], and two types of initial conditions have been applied: A fast top, i.e. $2\mathcal{V}/\mathcal{T} < 0.05$, and a purely precessing top, see e.g. [4]. For both cases the energy and the spatial component l_3 of the angular momentum are conserved within the iteration tolerance when the projection operator is included in front of the gradient of the gravitational potential in (11), and the second-order convergence is still retained in the presence of an external potential as illustrated in Fig. 3(b).

Conclusions

An energy and momentum conserving time-integration algorithm for rigid body rotations has been presented in terms of the four quaternions parameters and their conjugate momentum variables. It is illustrated that the two constraint conditions associated with the redundant parametrization are embedded in the equations of motions and do not require special attention apart from a projection of the external potential gradient. Furthermore, the role of the auxiliary inertia parameter has been revealed as a weighting factor on the normalization constraint and should be chosen large compared to the physical moments of inertia in order to ensure accurate satisfaction of the constraint condition.

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